WARZYN

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MEMORANDUM

August 20, 1990

TO: Robert Swale, RPM U.S. EPA Region V

FROM: Kevin Domack, Warzyn KJD
John Hurtenbach, Warzyn JRH

RE: Evaluation of chemical concentration data for use in the Baseline Risk Assessment at ACS
Job No. 60251.17

The evaluation of environmental data collected from the American Chemical Service Site (ACS) for use in the exposure assessment was initiated with the procedures outlined in Risk Assessment Guidance for Superfund, Interim Final, EPA/540-1-89/002 (RAGS) and "EPA Region III Guidance on Reporting and Handling of Chemical Concentration Data in Exposure Assessments", December 13, 1989 (Region III guidance).

In determining exposure point concentrations for media at a Superfund site the 95% upper confidence level of the arithmetic mean (UCLM) is applied. The 95% UCLM will be used in the Baseline Risk Assessment (BRA) as an estimate of the exposure point concentration for a particular medium (soil, water or air) unless this value is greater than the the maximum concentration detected on site. In this case, the maximum concentration detected on-site will be used as the estimate of the exposure point concentration instead of the 95% UCLM.

The site data has been divided into zones which represent discrete areas of contamination and points of human exposure. Where multiple rounds of data exist, each sample from each round will be considered an independent data point, and will be factored into the exposure point calculation as such. Field duplicate analyses will not be included as a second sample data point.

The initial examination of the data for these specific zones at ACS revealed a wide range of concentrations for the identified compounds. While some samples were relatively clean, other samples required dilutions ranging from 1:2 up to 1:1,000,000. These dilutions, while required for one or two compounds in a sample, elevated the Sample Quantitation Limit (SQL) for the remaining undetected compounds to correspondingly high values. How the non-detect values from diluted samples are treated when determining the 95% UCLM can bias the exposure concentration either high or low.

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While the two noted documents provided the basis for the evaluation of this data, it is felt that clarification of the procedure used in determining the value assigned to non-detects is required. The 3-step decision path presented in the Region III Guidance, combined with guidelines from RAGS, is used to address the data associated with this site.

Please notify Warzyn if this procedure does not meet with EPA approval. If Warzyn is not notified by Friday August 24, 1990, we will assume this procedure is acceptable to the EPA and proceed.

GENERAL CASE

The Region III Guidance and RAGS detail the general guidelines to evaluate data points for inclusion in the 95% UCLM. Any compound detected in any zone related sample for a given matrix is evaluated. All positive detects are included in the evaluation. Non-detects are evaluated and either assigned a value of zero or one-half the SQL, or are eliminated from the data set.

The Region III guidelines specifies that the Limit of Detection (LOD), as well as the Limit of Quantitation (LOQ), as used in the data evaluation be defined. The LOD is interpreted to be the instrument detection limit (the lowest concentration level that can be determined to be statistically different from a blank). The LOQ (the smallest concentration for which a quantitative result may be obtained with a specified degree of confidence) is interpreted to be equivalent to the Sample Quantitation Limit (SQL). The SQL is the product of the LOQ times correction factors for sample volume, percent moisture (for non-aqueous matrices), and any dilutions or concentrations beyond those specified in the method procedure.

The inorganics SOW specifies Contract Required Detection limits (CRDLs), which also have the same definition as SQLs. The Instrument Detection Limit (IDL) as well as the CRDL is reported for inorganic analytes. For metals and cyanide results, the IDL has the same definition as LOD. All analyte concentrations above the IDL are reported, and qualified as less than the CRDL but greater than or equal to the IDL.

The organics Statement of Work (SOW) for the Contract Laboratory Program (CLP) specifies Contract Required Quantitation Limits (CRQLs), which have the same definition as SQLs. The SOW does not require LODs to be reported for organic compounds. Volatile and semi-volatile compounds analyzed by Gas Chromatography/Mass Spectroscopy (GC/MS) that are present below the CRQLs are reported. Since the CRQL is higher than the LOD, it is possible to identify and quantitate compounds below the CRQL. These results are qualified as estimated. Pesticide/PCB compounds analyzed by Gas Chromatography

(GC) are not reported below the SQL. Since the LOD is not available for organic compound results, the SQL must be used instead. This is consistent with section 5.3.4 of RAGS.

For the purpose of this memorandum, SQL will be defined as the CRQL for all organic results, and as the IDL for all inorganic results. It represents the lowest known concentration that can be determined to be statistically different from a blank, given the available information about the data.

The following underlined scheme from the Region III guidance is used to determine which value for non-detects is used in calculating exposure concentrations.

1. Non-detects are to be evaluated for any compound which is present in a site related sample. For ACS, exposure concentrations are calculated for any compound that is detected in one or more samples.

2. Non-detects are to be evaluated as to whether it is reasonable to assume a compound may be present below the SQL based on site considerations. If so, a value of one-half the SQL for non-detects is used. This involves reviewing zone related samples for the presence of the compound or a related compound or set of conditions which could predict the presence of the compound. For ACS this process would be difficult due to the number of compounds present, the probable existence of sub-sites within a zone, and the wide range of concentrations found. As such, if a compound is found in any sample, it will be assumed that it reasonably may be present in related samples even though they may be qualified as not detected. The guidelines contained herein will then be used to determine what value, if any, to assign to these samples.

3. A determination is made as to whether a compound could reasonably be present in the sample based on an assessment of the chemical and physical characteristics of the compound and the sample matrix. If so, a value of one-half the SQL is used. For ACS, given the number of contaminants present and their potential interrelated properties, it is assumed that any detected compound could reasonably be present.

Benzene results from a zone of contamination at ACS illustrates the procedure used. Fourteen soil samples were analyzed for volatiles, with the following results for Benzene:

RESULTS (ug/kg)	SQL	1/2 SQL
710	6	3
6	6	3
550	1450	725
430	750	375
1400	750	375
1200	750	375
10	6	3
320	700	350
7,100,000	8,200,000	4,100,000
48,000	7,000	3,500
ND	6	3*
ND	6	3*
ND	6	3*
ND	750	375*

ND = non-detected

* = Used in conjunction with the positive results to calculate the exposure point concentration.

In this example, 10 of 14 samples had positive detects for Benzene. In this data set, it is apparent that benzene is present in the zone, and there is reason to suspect that it may be present in the undetected samples below the SQL. In this instance, for the benzene non-detects, one-half of the SQL is used for determination of the exposure concentration.

DETERMINING NON-DETECT VALUES FOR HIGHLY DILUTED SAMPLES

In the data set above, high levels of benzene, xylenes, or other volatile compounds were found in several samples at concentrations requiring significant dilutions in order to avoid saturating the GC/MS detector and exceeding the instrument's calibration range. Each individual sample's dilution is factored into the SQL, and raises the SQL for all the compounds in that sample. For example, the calibration range for benzene is 5 to 200 ug/kg. One sample required a dilution factor of 1400 in order to get benzene at 48,000 ug/kg within the calibration range. This raised the SQL for benzene to 7,000 ug/kg. The SQL for any other compound in this analysis is also multiplied by a factor of 1400.

Other volatile compounds present at levels below the high concentrations of benzene and xylene were found in this zone as well. For example 2-butanone was found in this zone at a maximum concentration of 210 ug/kg. 1/2 the SQL for 2-butanone from the highest diluted sample in the zone is 8,000,000 ug/kg. Inclusion of this and other similar non-detect values from highly diluted samples would significantly bias the exposure concentration.

Region III was contacted on 8-7-90 for further guidance on this issue. Roy Smith, a toxicologist at Region III, pointed out that it was within the RAGS to eliminate non-detect values from the data set in this situation, as specified in section 5.3.2. The section states:

> "if SQLs cannot be reduced...exclude the samples from the quantitative risk assessment if they cause the calculated exposure concentration to exceed the maximum detected concentration for a particular data set."

The 2-butanone results from the same fourteen sample points as above illustrates this point.

RESULTS (ug/kg)	SQL	1/2 SQL
73	12	6
190	12	6
210	12	6
21	12	6
140	12	6
ND	12	6*
ND	2900	1450
ND	1500	750
ND	1500	750
ND	1500	750
ND	1500	750
ND	1400	700
ND	14,000	7,000
ND	16,000,000	8,000,000

ND = non-detected

* = Used in conjunction with the positive results to calculate the exposure point concentration.

In this example, including all the non-detect 1/2 SQLs would result in a very large high bias. Thus, only non-detect 1/2 SQLs less than the highest positive detect (marked with an asterisk) are used. Since the maximum detected concentration is 210 ug/kg, only one of the nine non-detects would be included for 2-butanone. In evaluating this set of data, it seems reasonable not to include values (1/2 the SQL) that are from greater than 3 to greater than 38,000 times higher than the maximum detection in the zone of contamination.

DETERMINING NON-DETECT VALUES FOR COMPOUNDS WITH LOW POSITIVE VALUES

A third case appears in the same data set where the highest positive detect for a compound is below the SQL. This is possible in GC/MS data where the SQL is set above the Instrument Detection Limit; results

below the SQL are reported as "J" values and are estimated since they were not within the calibration range of the instrument. The qualitative identification of the sample is not an estimate, and the compound is considered to be present.

Including both the diluted and non-diluted sample non-detects would bias the exposure point concentration high in this case. The highly diluted sample values would be eliminated as shown in the previous example, and the non-diluted samples would be eliminated since it is unlikely they would be present. Section 5.3.3 of RAGS states "If there is reason to believe that the chemical is present in a sample at a concentration below the SQL, use one-half the SQL as a proxy concentration" and that "unless site-specific information indicates that a chemical is not likely to be present in a sample, do not substitute the value zero in place of the SQL". When the maximum detected concentration is below the SQL, it is reasonable to assume the chemical is not present in the non-detected sample. However, substituting zero for 1/2 the SQL would bias the exposure concentration low. We are suggesting for the ACS data that:

> samples should be excluded from the quantitative risk assessment if 1/2 the SQL is greater than the maximum detected concentration, or when using zero would bias the exposure concentration low.

The same data set is used. Here, 1,1,2-trichloroethane only had one sample out of fourteen with a positive detect.

RESULTS (ug/kg)	SQL	1/2 SQL
2	6	3
ND	6	3
ND	6	3
ND	6	3
ND	6	3
ND	1450	725
ND	750	375
ND	750	375
ND	750	375
ND	750	375
ND	6	3
ND	700	350
ND	7,000	3,500
ND	8,200,000	4,100,000

For this example, 1/2 the SQL for each non-detect is greater than the highest positive detect. Using a value of zero for the low non-detects, while not including the highly diluted non-detects, would bias the value

low. Only the detect is used. Again, in looking at this set of data, it would be unreasonable to include data at 1/2 the SQL for 1,1,2-trichloroethane given that the only positive detection is 2 ug/kg.

JAH/dlk/KJD
[dlk·108-91]
60251-MD

cc: P. Vaght
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